PCT WORLD INTELLECTUAL PROPERTY ORGANIZATION
International Bureau

INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(51) International Patent Classification 7 : G06F

A2

(11) International Publication Number: **WO 00/10067**

(43) International Publication Date: 24 February 2000 (24.02.00)

(21) International Application Number: PCT/US99/18302

(22) International Filing Date: 13. August 1999 (13.08.99)

(30) Priority Data:
60/096,425 13 August 1998 (13.08.98) US

(71) Applicant *(for all designated States except US)*: GEORGETOWN UNIVERSITY [US/US]; 3900 Reservoir Road, N.W., Washington, DC 20007 (US).

(72) Inventors; and
(75) Inventors/Applicants *(for US only)*: WU, Xiong-Wu [CN/US]; 7610 Savannah Street #103, Falls Church, VA 22043 (US). WANG, Shaomeng [US/US]; Apartment #309, 7540 Tremayne Place, McLean, VA 11102 (US).

(74) Agent: TESKIN, Robin, L.; Burns, Doane, Swecker & Mathis, L.L.P., P.O. Box 1404, Alexandria, VA 22313-1404 (US).

(81) Designated States: JP, US, European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE).

Published
Without international search report and to be republished upon receipt of that report.

(54) Title: SELF-GUIDED MOLECULAR DYNAMICS SIMULATION FOR EFFICIENT CONFORMATIONAL SEARCH

(57) Abstract

A method of forming a generated conformation of a molecular system comprising generating a molecular dynamics trajectory of said molecular system, wherein said trajectory is initiated by assigning to each atom in said molecular system a set of initial parameters comprising an initial velocity vector and an initial conformation wherein each atom in said molecular system is disposed in an initial position, and wherein said molecular dynamics trajectory is propagated by a computational procedure comprising: (a) calculating a current force exerted on each atom (i) by calculating a derivative of an energy function describing interactions between said atom (i) and other atoms in said molecule; (b) determining a guiding force g_i describing an average along a portion of said trajectory of a force exerted on said atom (i); (c) determining a current position and velocity of said atom (i) by ajusting said previous position and velocity according to the equation $m_i a_i = f_i$, wherein m_i is the mass of atom (i), a_i is an acceleration of atom (i) and f_i is a force obtained by adding said current force calculated in (a) and said guiding force determined in (b); (d) replacing said previous position and velocity of said atom (i) with said current position and velocity of said atom (i); (e) repeating steps (a) to (d) for one or more iterations to generate said trajectory; and (f) forming said generated conformation by disposing the atoms of said molecule in respective current positions obtained during a given iteration; and processing said generated conformation to determine a structural, energetic, thermodynamic or kinetic property of said molecular system.